Abstract Submitted
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A DFT based method for energy and information-entropic analysis in quantum confined atomic systems[1] SANGITA MAJUMDAR, AMLAN K ROY, IISER Kolkata — Atom trapped inside a cavity introduces fascinating changes in the observable properties. Here we report some preliminary theoretical results of the development and current status of a newly proposed DFT-based method in our laboratory, to address quantum confinement in atoms. This adopts a physically motivated non-variational, work-function-based exchange potential, along with a local parametrized simple Wigner functional and a nonlinear, gradient- and Laplacian-dependent functional. GPS method is used to construct an optimized non-uniformly discretized spatial grid for solving the non-relativistic KS differential equation. Exploratory results are presented for atoms and ions enclosed within impenetrable and penetrable spherical cages, along with other environments in both ground and excited states. That includes external potential in the form of harmonic confinement, atom/ion embedded in a plasma environment or in a fullerene cage. The exchange-only results are practically of Hartree-Fock quality. With inclusion of correlation; these are comparable to some of the multi-configurational calculations. Information theoretical quantities, such as Shannon entropy, Renyi entropy, Tsallis entropy, Fisher information,Onicescu energy, etc., are also presented in stated environment.

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